

A note on the convergence of the secant method for simple and multiple roots*

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To appear in **Applied Mathematics Letters**

Abstract

The secant method is one of the most popular methods for root finding. Standard text books in numerical analysis state that the secant method is super linear: the rate of convergence is set by the gold number. Nevertheless, this property holds only for simple roots. If the multiplicity of the root is larger than one, the convergence of the secant method becomes linear. This communication includes a detailed analysis of the secant method when it is used to approximate multiple roots. Thus, a proof of the linear convergence is shown. Moreover, the values of the corresponding asymptotic convergence factors are determined and are found to be also related with the golden ratio.

Keywords: Secant method, Convergence rate, Asymptotic behavior

AMS subject classification: 65H05

1 Introduction

The secant method is a variation of the Newton-Raphson method due to Newton himself [1]. The Newton-Raphson method converges quadratically to simple roots. Nevertheless, the convergence degenerates to linear when approximating a root with multiplicity m larger than 1. On the other hand, it is well known that the secant method is superlinear for simple roots. It has also been noticed that the super linear behavior is lost for multiple roots. This note recalls a compact proof of the convergence properties of the Newton-Raphson method and performs an accurate analysis of the secant method in front of multiple roots.

*This work was supported by the Ministerio de Ciencia y Tecnología, Spain, DPI2001-2204

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1.1 Assessing the convergence

The goal of an iterative solver for nonlinear scalar equations is to approximate α such that $f(\alpha) = 0$, being f a given function. The iterative method furnishes a sequence of approximations $\{x^0, x^1, x^2, \dots\}$. The analysis of the convergence of such method is based on characterizing the evolution of the error sequence $\{e^0, e^1, e^2, \dots\}$, where $e^k := \alpha - x^k$. The method is said to be convergent if

$$\lim_{k \rightarrow \infty} |e^k| = 0. \quad (1)$$

More precisely, the method is said to have convergence of order p if it exists λ such that

$$\lim_{k \rightarrow \infty} \frac{|e^{k+1}|}{|e^k|^p} \leq \lambda, \quad (2)$$

where λ is denoted Asymptotic Error Constant (AEC) [3]. When $p = 1$, convergence is reached only if $\lambda \leq 1$ (linear convergence).

Assuming that the method is convergent, that is Eq. (1) holds, the order of convergence of the method is studied using the following truncated Taylor expansions:

$$f(x^k) = -f'(\alpha)e^k + \frac{1}{2}f''(\alpha)(e^k)^2 + O(|e^k|^3) \quad (3)$$

(recall that $f(\alpha) = 0$) and

$$f'(x^k) = f'(\alpha) - f''(\alpha)e^k + O(|e^k|^2) \quad (4)$$

If α is of multiplicity $m > 1$ (that is, $f(\alpha) = f'(\alpha) = \dots = f^{m-1}(\alpha) = 0$), Eq. (3) is replaced by

$$f(x^k) = \frac{(-1)^m}{m!} f^{(m)}(\alpha) (e^k)^m + O(|e^k|^{m+1}) \quad (5)$$

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and Eq. (4) is replaced by

$$f'(x^k) = \frac{(-1)^{m-1}}{(m-1)!} f^{(m)}(\alpha) (e^k)^{m-1} + O(|e^k|^m). \quad (6)$$

1.2 Convergence of Newton-Raphson method

The analysis of the Newton-Raphson method is recalled because both the framework and the results are very similar to those of the secant method. Newton-Raphson iteration generates a sequence of approximations using the following expression:

$$x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)}. \quad (7)$$

The corresponding expression for the error is

$$e^{k+1} = e^k - \frac{f(x^k)}{f'(x^k)} \quad (8)$$

The analysis of the behavior of the method for simple roots ($f'(\alpha) \neq 0$) is performed replacing Eqs. (3) and (4) in Eq. (8), that is,

$$e^{k+1} = \frac{-\frac{1}{2}f''(\alpha)(e^k)^2 + O(|e^k|^3)}{f'(\alpha) - f''(\alpha)e^k + O(|e^k|^2)}. \quad (9)$$

Assuming that the method is convergent, in the asymptotic range (for $k \rightarrow \infty$) the higher order terms in Eq. (9) are neglected. In the following the “asymptotic equality” is denoted by \asymp and is used when the equality holds for $k \rightarrow \infty$. Then,

$$e^{k+1} \asymp \frac{-\frac{1}{2}f''(\alpha)(e^k)^2}{f'(\alpha)} \quad \text{and} \quad \lim_{k \rightarrow \infty} \frac{|e^{k+1}|}{|e^k|^2} = \frac{|f''(\alpha)|}{2|f'(\alpha)|}. \quad (10)$$

Therefore the convergence is quadratic ($p = 2$).

On the contrary, when the root is of multiplicity $m > 1$, the analysis is performed replacing Eqs. (5) and (6) in Eq. (8), that is,

$$e^{k+1} = e^k + \frac{\frac{(-1)^m}{m!}f^{(m)}(\alpha)(e^k)^m + O(|e^k|^{m+1})}{\frac{(-1)^{m-1}}{(m-1)!}f^{(m)}(\alpha)(e^k)^{m-1} + O(|e^k|^m)} = e^k \frac{1 - 1/m + O(|e^k|)}{1 + O(|e^k|)}. \quad (11)$$

Then, in the asymptotic range,

$$e^{k+1} \asymp \left(1 - \frac{1}{m}\right) e^k \quad \text{that is} \quad \lim_{k \rightarrow \infty} \frac{|e^{k+1}|}{|e^k|} = 1 - \frac{1}{m}. \quad (12)$$

Consequently, for roots of multiplicity m , the method exhibits linear convergence with AEC equal to $1 - 1/m$. In particular, for double roots ($m = 2$) the AEC is $1/2$.

The same kind of analysis is performed to derive the convergence properties of the secant method for both simple and multiple roots.

2 Analysis of the secant method

The secant method may be seen as a variation of the Newton-Raphson method. The derivative in Eq. (7) is replaced by an incremental rate:

$$f'(x^k) \approx \frac{f(x^k) - f(x^{k-1})}{x^k - x^{k-1}}. \quad (13)$$

Thus, the secant iteration is obtained replacing Eq. (13) in Eq. (7), that is

$$x^{k+1} = \frac{x^{k-1}f(x^k) - x^kf(x^{k+1})}{f(x^k) - f(x^{k-1})}. \quad (14)$$

The corresponding sequence of errors is generated by the following expression:

$$e^{k+1} = \frac{e^{k-1}f(x^k) - e^kf(x^{k+1})}{f(x^k) - f(x^{k-1})}. \quad (15)$$

2.1 Behavior for simple roots

Let α be a simple root ($f'(\alpha) \neq 0$). Assume that the method is convergent (that is, Eq. (1) holds). Introducing the expansion of Eq. (3) and the corresponding version for $f(x^{k-1})$ in Eq. (15) one gets

$$e^{k+1} = \frac{1/2f''(\alpha)e^ke^{k-1} + O(|e^k|^4)}{f'(\alpha) + 1/2f''(\alpha)(e^k + e^{k-1}) + O(|e^k|^3)}, \quad (16)$$

where, since convergence is assumed, the term $O(|e^{k-1}|^r)$ dominates the term $O(|e^k|^r)$ for $r = 3$ and $r = 4$. Then, the asymptotic version of Eq. (16) (for $k \rightarrow \infty$) is

$$e^{k+1} \asymp \frac{f'''(\alpha)}{2f'(\alpha)} e^k e^{k-1}. \quad (17)$$

Extracting the logarithm of Eq. (17) and introducing the notation $a^k := \ln e^k$, yields

$$\ln e^{k+1} \asymp C + \ln e^k + \ln e^{k-1} \quad \text{and} \quad a^{k+1} \asymp C + a^k + a^{k-1}, \quad (18)$$

where $C := \ln \left(\frac{f'''(\alpha)}{2f'(\alpha)} \right)$. That is, the sequence $\{a^k\}$ ($k = 1, 2, \dots$) is a Fibonacci numerical sequence.

Assume the following asymptotic behavior

$$a^{k+1} \asymp \Phi a^k + \beta \quad (19)$$

Then, imposing (18) for k and $k+1$, the only possible (positive) values for Φ and β are found to be

$$\Phi = \frac{\sqrt{5}+1}{2} \approx 1.618 \quad \text{and} \quad \beta = \frac{C}{\Phi} \quad (20)$$

Of course, Φ is the gold number related with the Fibonacci sequences.

To verify that the assumption introduced in Eq. (19) is valid in the asymptotic range, we introduce the error associated with this hypothesis, that is

$$\varepsilon^{k+1} := a^{k+1} - (\Phi a^k + \beta). \quad (21)$$

We characterize the evolution of the error in the assumption of Eq. (19) replacing Eq. (21) in Eq. (18). That yields

$$\varepsilon^{k+1} = -\frac{\varepsilon^k}{\Phi}. \quad (22)$$

That is, the error ε^k tends linearly to 0 because $1/\Phi \approx 0.618 < 1$. Consequently, Eq. (19) tends to be verified asymptotically.

Thus, in the asymptotic range, Eq. (19) holds and therefore

$$e^{k+1} \asymp \exp(\beta) (e^k)^\Phi, \quad (23)$$

that is, the secant method exhibits superlinear convergence (convergence of order $p = \Phi > 1$) with AEC $\lambda = \exp \beta = \left(\frac{f''(\alpha)}{2f'(\alpha)} \right)^{1/\Phi}$. The proof of this property is classical but not unique, see [2] for two different options and a discussion.

2.2 Behavior for multiple roots

Let α be a root with multiplicity $m > 1$.

Introducing the expansion of Eq. (5) and the corresponding version for $f(x^{k-1})$ in Eq. (15) one gets

$$e^{k+1} = \frac{e^{k-1} (e^k)^m - e^k (e^{k-1})^m + O(|e^{k-1}|^{m+2})}{(e^k)^m - (e^{k-1})^m + O(|e^{k-1}|^{m+1})}, \quad (24)$$

where, since convergence is assumed, the term $O(|e^{k-1}|^r)$ dominates the term $O(|e^k|^r)$ for $r = m+1$ and $r = m+2$.

2.2.1 Double roots ($m = 2$)

For double roots, neglecting the terms $O(|e^{k-1}|^3)$ and $O(|e^{k-1}|^4)$, Eq. (24) becomes

$$e^{k+1} \asymp \frac{e^{k-1} e^k}{e^k + e^{k-1}}, \quad (25)$$

Eq. (25) may be rewritten as

$$\frac{1}{e^{k+1}} \asymp \frac{1}{e^k} + \frac{1}{e^{k-1}}. \quad (26)$$

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Thus, the sequence of $1/e^k$, $k = 0, 1, 2, \dots$ is a Fibonacci sequence (with $C = 0$). Then, according to the previous section, the following expressions hold in the asymptotic regime:

$$\frac{1}{e^{k+1}} \asymp \Phi \frac{1}{e^k} \quad \text{and therefore} \quad e^{k+1} \asymp \frac{1}{\Phi} e^k. \quad (27)$$

Recall that $1/\Phi = 1 - \Phi \approx 0.618$. Thus, for double roots, the secant method exhibits linear convergence with AEC equal to $1 - \Phi$.

2.2.2 Multiplicity larger than 2 ($m > 2$)

The superlinear converge is lost for double roots. Then, for $m > 2$, the secant method is also assumed to be linear with AEC equal to λ . Thus, in the asymptotic regime, the following equality holds

$$e^{k+1} \asymp \lambda e^k. \quad (28)$$

Multiplicity (m)	Order (p)	AEC (λ)
1	2	$\left \frac{f''(\alpha)}{2f'(\alpha)} \right $
2	1	1/2
3	1	2/3
\vdots	\vdots	\vdots
m	1	$1 - 1/m$

Table 1: Summary of the convergence behavior of Newton-Raphson method

Multiplicity (m)	Order (p)	AEC (λ)
1	$\Phi \approx 1.618$	$\left \frac{f''(\alpha)}{2f'(\alpha)} \right ^{1/\Phi}$
2	1	$\lambda = 1/\Phi \approx 0.618$
3	1	$\lambda \approx 0.755$
\vdots	\vdots	\vdots
m	1	$0 < \lambda < 1$ such that $\lambda^m + \lambda^{m-1} - 1 = 0$

Table 2: Summary of the convergence behavior of the secant method

An equation for λ is recovered introducing Eq. (28) in Eq. (24) and neglecting higher order terms:

$$\lambda^2 = \frac{\lambda^m - \lambda}{\lambda^m - 1} \Rightarrow \lambda(\lambda - 1)(\lambda^m + \lambda^{m-1} - 1) = 0. \quad (29)$$

This polynomial equation has a unique root such that $0 < \lambda < 1$. This root is slightly lower than (and almost equal to for large m) $(1)^{1/m}$. Obviously for $m = 2$ the value of the previous section is recovered and for $m = 3$ an analytical expression is also available

$$\lambda = \frac{1}{6} \left(100 + 12\sqrt{69} \right)^{1/3} + \frac{2}{3(100 + 12\sqrt{69})^{1/3}} - 1/3 \approx 0.7548776667.$$

3 Conclusion

The analysis performed in this work proofs that the convergence behavior of the secant method is analog to behavior of the Newton-Raphson method. The convergence properties of both methods are summarized in tables 1 and 2. The analysis shows that the secant method loses the superlinear behavior when the root has multiplicity larger than one. Moreover, the AEC is characterized as one of the solutions of a polynomial equation of degree m .

References

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